

H. S. Köhler ¹

Physics Department, University of Arizona, Tucson, Arizona 85721, USA

Abstract

The energy-spectrum of two point-like particles interacting in a 3-D isotropic Harmonic Oscillator (H.O.) trap is related to the free scattering phase-shifts δ of the particles by a formula first published by Busch et al. It is here used to find an expression for the *shift* of the energy levels, caused by the interaction, rather than the perturbed spectrum itself. In the limit of high energy (large quantum number n of the H.O.) this shift is shown to be given by $-2\frac{\delta}{\pi}$, also valid in the limit of infinite as well as zero scattering length at all H.O. energies.

Numerical investigation shows that the shifts differ from the exact result of Busch et al, by less than $< \frac{1}{2}\%$ except for $n = 0$ when it can be as large as $\approx 2.5\%$.

This approximation for the energy-shift is well known from another exactly solvable model, namely that of two particles interacting in a spherical infinite square-well trap (or box) of radius R in the limit $R \rightarrow \infty$, and/or in the limit of large energy. It is in this context referred to as the *phase-shift approximation*.

It can be (and has been) used in (infinite) nuclear matter calculations to calculate the two-body effective interaction in situations where in-medium effects can be neglected. It has also been used in expressing the energy of free electrons in a metal.

1 Introduction

Recent years has seen a tremendous progress in the ability to study the physics of atoms trapped in confined optical lattices. A significant development has been the tuning of the interactions (scattering lengths) between the particles via Feshbach resonances.[1] A further important achievement is the ability to confine just a few atoms in a potential well or trap.[2] The situation of a few particles confined in this fashion is also encountered in other areas of physics. One old problem in nuclear physics is for example that of two or more nucleons 'outside' a closed shell. The recent experimental research in atomic physics that enables a control of interactions as well as the environment represented by the trap has stimulated theoretical studies of this basic quantum-mechanical problem: two or more particles interacting while trapped in some specified potential well.

In this paper ² the investigation is restricted to two particles in either a 3-dimensional H.O. trap or in a spherical square-well trap. Of particular interest in a study of this kind is of course the two-body interaction between the particles. It can be represented by some potential model e.g. pseudo-potential [13, 21] or chiral effective field theory potential[18].

It is however found that the interactions, under specific assumptions, can be related to scattering data and this is the route taken in this report.

1.1 3-D H.O. well

An expression first derived by Busch et al [17] relates the *energy-spectrum* of two point-like particles, interacting in a 3-D Harmonic Oscillator (H.O.) well, to scattering phase-shifts. The derived formula is restricted to point-like particles, meaning that the range of the interaction has to be short compared to the size of the trap and is then the solution of an exactly solvable model. The pointlike interaction implies that the relative angular momentum $l = 0$. The formula has been extended to $l > 0$ assuming that the range of the interaction is still small. [19]

In the present work, restricted to $l = 0$, the expression for the two-particle energy spectrum as derived in ref. [17] is used to find the *shifts* in energy-levels from the non-interacting to the interacting spectrum. It is shown that these shifts converge to the phase-shift approximation for large H.O. quantum-numbers n and for small as well as large scattering lengths. Calculations, shown in Sect. 2, moreover show that the phase-shift approximation and the 'exact' result for the two-body spectrum obtained by Busch et al. give practically indistinguishable results.

The good agreement with the phase-shift approximation for the two-body spectrum may be unique to the H.O. trap.

¹e-mail: kohlers@u.arizona.edu

²A preliminary version of this report is found in ref. [3]

For comparison, in the similar case of two particles interacting in a spherical square well the calculations presented in Sect. 3 shows that the phase-shift approximation is viable only in the limit of small (in units of box-radius) scattering lengths and large n -values and it is in general a much worse an approximation than it is for the H.O.

1.2 Spherical square-well

If the trap is a spherical square-well (or box) the shift in energy spectrum due to the two particle's mutual interaction can, as shown below in Sect. 3, easily be obtained without reference to a potential model.[10, 11] In the limit of a large size of the box this shift is $\propto \delta(k)$, the scattering phase-shift at momentum k . (Only angular momentum $l = 0$ is considered here although most results are also valid for all values of l .)

A more elaborate but instructive method of obtaining the energy-shift was used in early attempts of developing a many-body theory of nuclei. Brueckner initially assumed the in-medium (effective) two-body interaction to be $\propto \tan \delta(k)$. [4] The initial problem studied was that of an 'infinite' system of nuclear matter for the purpose of calculating binding energy and saturation properties of this system. The $\tan \delta(k)$ approximation came from the assumption that the Reactance matrix [5], could be used as an approximation for the in-medium interaction in the many-body problem. (The diagonal part of this matrix is $\propto \tan \delta(k)$). The definition of the Reactance matrix involves a principal value integration over a *continuous* spectrum. It was assumed that the numerical summation over the closely spaced level-spectrum of nucleons in a very large ('infinite') box would give an equivalent result. This assumption was substantiated by Reifman and DeWitt[6]. It was however soon realized to be incorrect. Several authors (one of them DeWitt) showed that the correct limit for two particles in a big box would yield an in-medium interaction $\propto \delta(k)$ rather than $\tan \delta(k)$. [7, 8, 9] ³

The Reactance matrix is part of scattering theory. The nuclear matter problem assumes a box, although large but still finite with boundary conditions different from that of scattering theory. The proofs in the papers referred to above differ, but the essential point is that the integration over the continuous spectrum vs the summation over the discrete spectrum of particles in a box differ, even though the level-spacing in a big box goes towards zero as the box-size increases. The principal value integration relates to the scattering problem with boundary conditions different from that for a box where the wave-functions are zero at the edge of the box even in the limit of the box being 'infinitely' large.

The exact statement of the results in the referenced papers is that the energy-shift Δ due to the interaction of two-particles confined in a spherical box in the limit when the size of the box approaches infinity is given by

$$\Delta = S \times dE \quad (1)$$

where dE is the spacing between the levels of the unperturbed spectrum and ⁴

$$S = -\frac{\delta(k)}{\pi}. \quad (2)$$

This energy shift implies that the *diagonal* part of the 'effective' interaction in a big box is given by

$$V_{eff}(k) = 4\pi \frac{\delta(k)}{k} \quad (3)$$

In nuclear matter studies (implying an infinite box) this has been referred to as the 'phase-shift approximation' a term adopted here. It was for example used in early calculations on the neutron-gas[14, 15]. Many-body calculations do in general also require *off-diagonal* elements of the 'interaction, as in the calculation of the Brueckner reaction-matrix. In some early nuclear matter studies, these were obtained by assuming V_{eff} to be a separable interaction with the diagonal given by eq. (3).[16].

It is of interest to compare the energy-shifts in a *finite* size box with those of the H.O. trap. Results of these calculations are shown in Sect. 3.

2 3-D Harmonic Oscillator Well

Units of energy and length are here chosen to be $\hbar\omega$ and $a_o = \sqrt{\hbar/m\omega}$ respectively. The total energy for two non-interacting particles with zero angular momentum in a 3-D H. O. well is then $E_{tot} = E_0 + E_{cm} = 2n + 3$ ($n = 0, 1, 2, \dots$). Assuming the center-of-mass energy to be $E_{cm} = \frac{3}{2}$ the energy of relative motion is $E_0 = 2n + \frac{3}{2}$.⁵

³For small values of δ and at low density this might not make any difference but with $\delta \approx \pi/2$ (large scattering length), a situation often discussed in recent works, it obviously does.

⁴It was pointed out by DeWitt[8], after a comment by Brueckner that the result may be different for a box other than spherical.

⁵Only the dependence of the quantum-number of relative motion is relevant for the following

With the particles interacting, $E_0 \rightarrow E$ and with $\eta = 2E$ the energy spectrum is obtained from [17, 20]

$$\tan \delta(k) = -\frac{\sqrt{\eta}\Gamma[(1-\eta)/4]}{2\Gamma[(3-\eta)/4]} \quad (4)$$

where $k = \sqrt{\pi/2}/a_o$.

This expression for the energy-spectrum of two particles trapped in a H.O. well has already played an important role in interpreting experimental data in atomic physics. (E.g. refs.[25, 26]) It is cited in numerous recent articles related to nuclear structure.(E.g. ref. [21, 18]). It has been extended to relative angular momenta $l > 0$ by Suzuki et al [19].

It is here recast in a different form to explicitly show the energy-shifts $\Delta = E - E_0$ incurred by the two-body interaction. One finds

$$\eta = 4n + 3 + 2\Delta$$

. After substitution in eq. (4) and using the reflection formula for Γ -functions [22]

$$\Gamma(x) = \frac{\pi}{\Gamma(1-x)\sin(\pi x)} \quad (5)$$

one finds

$$\tan \delta(k) = -A(z) \tan\left(\frac{\Delta}{2\pi}\right) \quad (6)$$

or

$$\Delta = -\frac{2}{\pi} \arctan \frac{\tan(\delta(k))}{A(z)} \quad (7)$$

where

$$A(z) = \frac{\sqrt{z - \frac{1}{4}}\Gamma(z)}{\Gamma(z + \frac{1}{2})} \quad (8)$$

with

$$z = n + \Delta/2 + 1. \quad (9)$$

Eq. (7) is equivalent to eq. (4), first derived by Busch et al [17] although here rewritten in terms of the shift Δ instead of the energy $E = \eta/2$. Of particular interest here is the function $A(z)$.

Fig. 1 shows a rapid convergence of this function to its asymptotic value, i.e. $A(z) \rightarrow 1$ for increasing values of z , and in this limit eq. (7) reduces to eq.(2), referred to as the phase-shift-approximation.⁶

This also occurs, irrespective of the the value of $A(z)$, when $\delta(k) = 0$ and more importantly when $\delta(k) = \pm \frac{\pi}{2}$ in which case $\Delta = \mp 1$, a well-known result.[17, 20].

A correction $d\Delta$ to the phase-shift approximation of Δ (i.e. for values of z when $A(z) \leq 1$) is obtained from

$$d\Delta \approx -\frac{1}{\pi}(1 - A^{-1}(z))\sin(2\delta) \quad (10)$$

It is damped with decreasing values of $\sin 2\delta$ and goes to zero when $\delta = \pm \frac{\pi}{2}$ (and when $\delta = 0$) in accordance with above.

The left part of Fig. 2 shows the difference between the energy shifts calculated by eq. (7), and the phaseshift-approximation, eq. (2), respectively for H.O. Quantum-numbers $n = 0, 1$ and 2 . Results are shown as a function of scattering length a in units of a_o . The difference (error) is seen to decrease rapidly with increasing n and (as also shown above) with increasing value of $|a|$. The peaks are a result of the competition between the $A(z)$ and $\sin 2\delta$ terms respectively shown in eq. (10). The right part of the Fig. 2 shows the same differences but in % of the exact result again showing the rapid decrease with increasing values of n and with $|a|$. One finds larger differences for $n = 0$, while appreciably smaller for $n = 1$ and $n = 2$. This is of course related to the function $A(z)$. The smallest value of this function is for the smallest value of $z = \frac{1}{2}$ (see Fig. 1), which occurs for $n = 0$ $S = -\frac{1}{2}$, $n = 1$ $S = -\frac{3}{2}$ etc.

⁶Using the asymptotic formula for the Γ -function in ref.[22] one finds $A(z) \rightarrow \sqrt{\frac{z-\frac{1}{4}}{z}}$, indicating an appreciably slower convergence to the asymptotic value than the exact calculation that is shown in Fig. 1.

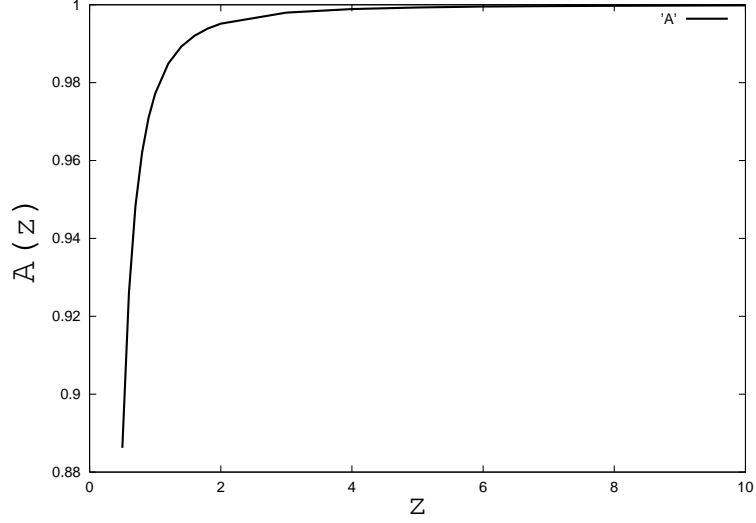


Figure 1: Function $A(z)$ defined in the text. Notice the asymptotic convergence of $A(z) \rightarrow 1$.

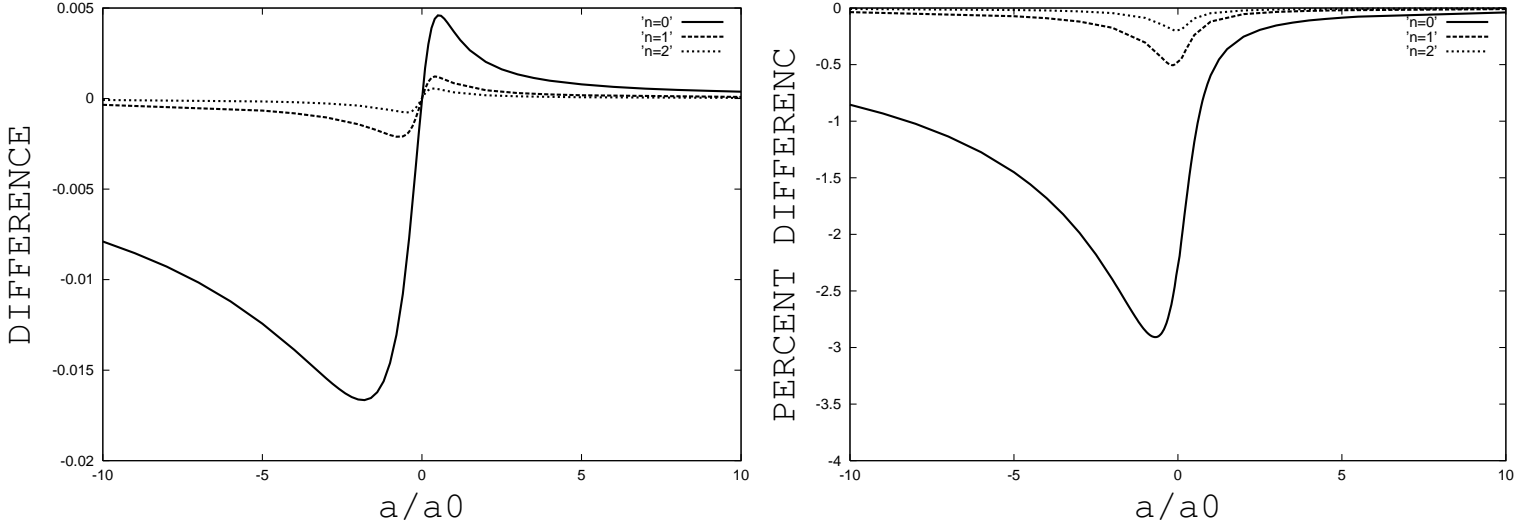


Figure 2: Curves to the left show the differences between energy-shifts calculated exactly, eq. (7) and by the phase-shift approximation (2) for two-particles in a H.O. trap for quantum-numbers $n = 0, 1$ and 2 , with $n = 0$ showing the largest difference. To the right is shown the same differences but expressed in percent. A comparison with the similar plot in Fig. 4 for the square well trap shows that the convergence with n is faster in this case.

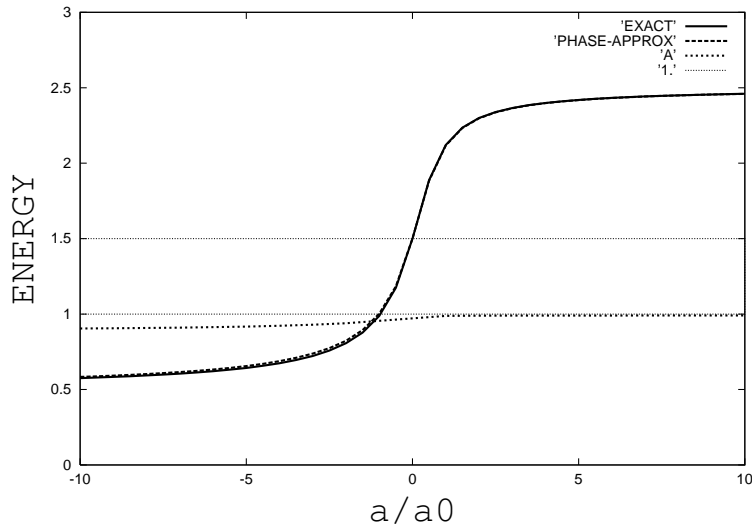


Figure 3: The solid line(s) show(s) the exact (eq. (4) two-body energy as a function of scattering length and also from the phase-shift approximation. The two lines practically coincide. A slight difference may be seen for negative scattering lengths. The comparison is for the worst scenario, the lowest H.O. energy, i.e. $n = 0$. Compare with Fig. 2 that shows the difference between the two curves. The broken line shows the function $A(z)$, eq. (1), where z is obtained from eq. (9). It is seen to converge towards $A(z) = 1$ for positive scattering lengths. The non-interacting H.O. energy is here $n + \frac{3}{2} = 1.5$.

The largest discrepancy is consequently expected to be found for $n = 0$ and for $a < 0$, where the shift is negative. The comparison between the exact result given by eq. (4) and the phase-shift approximation for this worst case is shown in Fig. 3. It shows practically complete overlap between the two curves even for this worst case. The 'correcting' factor $A(z)$ is also shown in this figure. It is seen that $A(z) \approx 0.9$ for negative scattering lengths but approaches the value $A(z) = 1$ for positive scattering lengths which is consistent with eq. (9). For comparison, calculations show that $A(z) \leq 0.991$ when $n = 1$ and with complete overlap between exact and the approximate results.

The conclusion is that the phase-shift approximation for the effective interaction applies equally well or even better in the H.O. case than it does in the square-well case shown below in Sect. 3. Again, of course, in a many body environment (three or more particles) also off-diagonal elements are needed. J. Rotureau [21] solves this problem by generating an interaction by a unitary transformation of the H.O. two-particle spectrum given by eq. (4).

A main result of this investigation is that the energy spectrum of two particles interacting in a H.O. trap can be simply constructed from the free-scattering phase-shifts as follows:

$$E(a) = E_0 - 2 \frac{\delta(k)}{\pi} \quad (11)$$

where E and E_0 are the perturbed and unperturbed levels respectively with $k = \sqrt{E(a)}$ and $\tan(\delta(k)) = -ak$.

As written, this result refers to two particles with point-like interactions and angular momentum $l = 0$. It can be extended to $l > 0$ but is then expected to be less accurate, as is also the case with the original formula eq. (4).

3 Spherical Square Well

It is of interest to compare the above result obtained with a H.O. trap with that of two particles in a spherical box of finite size as this may better correspond to some experimental setups.

The problem of two particles interacting in a box of *infinite* size was considered by several authors [10, 11, 7, 8, 9] referred to in the Introduction. with the result given by eq. (2), the phase-shift approximation. The special interest was, at the time, that of nuclear matter, a system of nucleons in a large but finite enclosure or of free electrons in a metal.

It is of interest to compare the result obtained with a H.O. trap with that of two particles in a spherical box of *finite* size. This may better correspond to some experimental setups.

The simplest solution [10, 11] of the problem at hand is to explicitly consider the wave-functions of the two particles in this box. It is an example of an exactly solvable model in quantum mechanics.[12] Considering only s -states, the radial wavefunctions of free non-interacting particles are (easily extended to angular momentum $l > 0$)

$$\Psi(r) \propto \frac{1}{r} \sin(k^{(0)}r) \quad (12)$$

With the two particles interacting, the wave-function outside the range of the interaction (assumed $\ll R$ or 'pointlike') is:

$$\Psi(r) \propto \frac{1}{r} \sin(kr + \delta(k)) \quad (13)$$

The boundary condition implies that wave-functions vanish at the boundary of the sphere. With units of energy and length chosen to be $\hbar^2/2m$ and well-radius R respectively one finds for the non-interacting case

$$k_n^{(0)} = n\pi \quad (14)$$

and for the interacting case

$$k_n + \delta(k_n) = n\pi \quad (15)$$

The spacing between unperturbed levels is

$$dE = 2n\pi^2$$

The energy shift is

$$\Delta = k_n^2 - k_n^{(0)2} = -\delta(k_n)(k_n + k_n^{(0)})$$

so that by eq. (1)

$$S = -\left(1 - \frac{\delta(k_n)}{2n\pi}\right) \frac{\delta(k_n)}{\pi} \quad (16)$$

showing that for large n and/or small δ

$$S \rightarrow -\frac{\delta(k_n)}{\pi}$$

which is the phase-shift approximation (2).

Fig. 4 shows the corrections $\frac{\delta(k_n)^2}{2n\pi^2}$ to the phase-shift approximation as a function of scattering length a and for some indicated values of quantum-number n .

The phaseshift is here a function of a and k_n by eq. (15) which is solved selfconsistently.

A comparison with the analogous result for the H.O. in Fig. 2 shows notable differences. While the largest deviation from the phase-shift approximation in the H.O. case is 3% (and typically much smaller), it is in the square well case seen to be as large as 30%. In the H.O. the largest error is for small scattering lengths while the error goes to zero for large scattering lengths. This is opposite to the situation encountered for the square well. Fig. 4 does however show the known result that $S \rightarrow -\frac{\delta(k)}{\pi}$ when $a/R \rightarrow 0$ [10, 11, 7, 8, 9].

Fig. 5 shows the two-body spectra calculated exactly compared with those obtained in the phase-shift approximation. The agreement between the the two sets of curves increases with increasing n as well as increasing R , i.e. size of the box but a comparison with Fig. 3 shows that the approximation works better in the H.O. case for the low-lying states.

4 Summary

The validity of the phase-shift approximation, $\Delta = -\frac{1}{\pi}\delta(k)dE$ for the energy-shift due to the interaction of two particles in a trap, where $\delta(k)$ is the free particle scattering phase-shift and dE the energy-level spacing of the unperturbed spectrum, has been investigated.

The traps considered were a 3-D H.O. and a spherical infinite square well (box). The square-well case was treated a long time ago as referenced above, with the main emphasis on the large size limit of the box with the result expressed by eq. (2), the phase-shift approximation. Somewhat of a surprise was the finding that a not

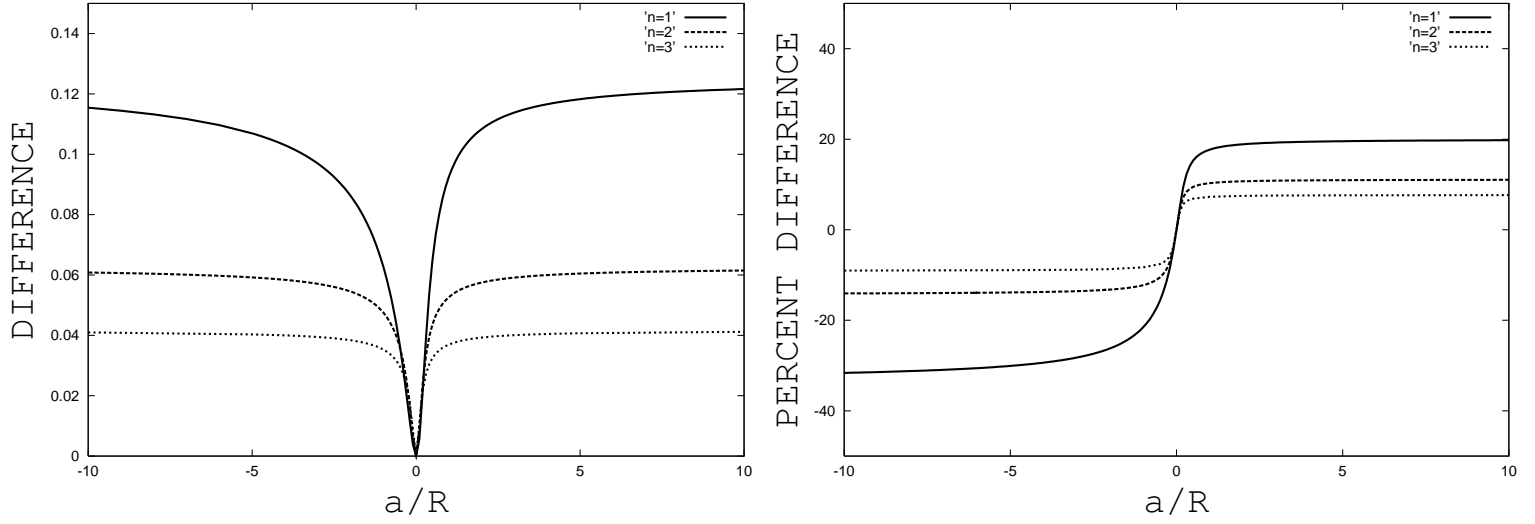


Figure 4: Curves to the left show corrections to the phase-shift approximation for two-particles in a spherical square well trap for quantum-numbers $n = 1, 2$ and 3 , with $n = 1$ showing the largest difference. To the right is shown the same differences but expressed in percent.

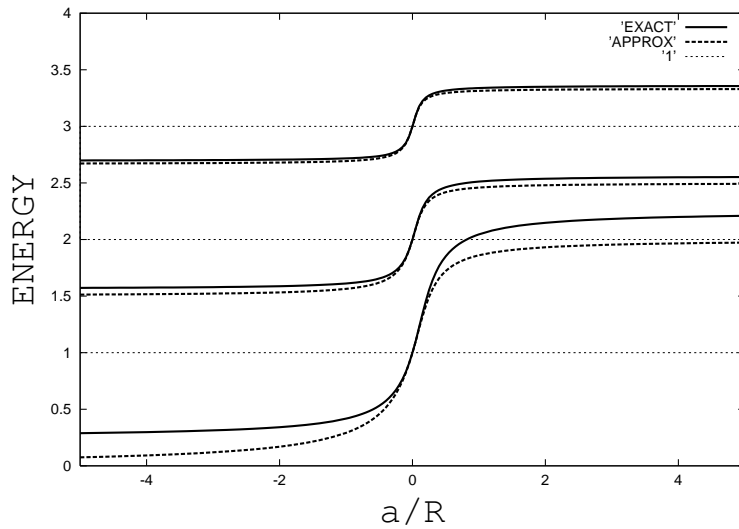


Figure 5: The solid lines show the exact two-body spectra for $n = 1, 2$ and 3 , while the broken lines show the result of the phase-shift approximation. The energies are normalised to the uncorrelated energies.

only somewhat similar situation exists for the H.O. trap but that the approximation is so much more accurate for this trap in the region of trap parameters of interest for finite systems. Eq.(11) can therefore be considered as an alternative to the formula of Busch et al [17]. In addition to being simple to use for calculating the two-body spectra in the H.O. it can also very simply be used to extract phase-shifts from experimental data.

The differences between the results for the two respective traps are seen by comparing Fig. 2 for the H.O.trap with Fig. 4 for the square-well trap. While in the square well case, the differences (errors) by using the phase-shift approximation are as large as 30%, the differences are much smaller and even practically zero in the H.O. case. The accuracy of the approximation in the H.O. case is also seen in Fig. 3 with curves practically overlapping even in the worst case, $n = 0$. For comparison, the scenario is rather different in the square well case shown by Fig. 5 where for the low-lying states the approximation is only valid for small values of a/R .

Another difference between the H.O. and the box results is that, with $a \rightarrow \pm\infty$ the phase-shift approximation becomes perfect in the H.O. case while this is not so in case of the box. In both cases the approximation becomes good for small values of the scattering-lengths, which is not surprising as the Born approximation would then be applicable.

The results presented here were for zero-range potentials, i.e. for zero effective range i.e. with $\tan\delta(k) = -ka$. Jonsell [20] found the finite range-corrections to be small in the H.O. case. The 'small' range is of course in relation to the physical size of the system, i.e. the length parameters defined above. This subject was also the subject of a recent publication.[23]

This investigation can be extended to angular momenta $l > 0$.

The question arises of course whether the phase-shift approximation has a more general validity e.g. for two particles in a *non-spherical* atomic nucleus or for particles in a cubical box. It was however already illustrated above that the situation is rather different in the 3-D H.O. case compared to the case of a spherical well. The conceptual differences between scatterings and interactions in the spherical vs cubical box was already pointed out by DeWitt in a detailed discussion of this matter. Quote[8]: *Only the spherical box (with spherical waves) is suitable for establishing a connection between single scattering processes and discrete spectrum theory....*but the problem of two atoms in an anisotropic H.O. trap was considered in ref. [27]. A related problem that of the relation between the energy spectrum and scattering phases of two particles in a cubical box but with *periodic* boundary conditions shift was however solved by Lüscher[24] . but the problem of two atoms in anisotropic H.O. trap was considered in ref. [27].

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